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Validation and Uncertainty Quantification of Hyperspectral Image Modeling

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INTRODUCTION

Identifying and applying appropriate validation and uncertainty quantification (V/UQ) methods is instrumental in strengthening the validity and scientific rigor of predictive modeling of the hyperspectral imaging (HSI) observables associated with solid particulate materials. Validating these predictive models and quantifying uncertainties inherent in the modeling process presents a significant research challenge.

In this paper, we present techniques for validating physics-based models that predict HSI observables of solid particulate materials and characterizing model uncertainties. We are employing a hierarchical V/UQ approach by designing physical experiments and comparing the experimental results with the outputs of computational predictive models [1]. We illustrate this approach by comparing a model for the reflectance of a particulate material to the reflectance spectrum acquired on a well-characterized particulate deposit. By validating physical models with experimental data at various scales, and characterizing and quantifying uncertainties in the modeling process, we anticipate that incorporation of V/UQ techniques will elevate the level of confidence stakeholders have in model utilization and model outputs.

VALIDATION/UQ PROCESS

The validation process that we are incorporating is shown in Fig. 1. The key elements of this process are verification [2], uncertainty quantification (UQ), validation (or comparison), and model maturity [3]. For this paper, the primary focus is on UQ, including calibration, sensitivity analysis (SA), and uncertainty analysis (UA), shown in the light blue shaded boxes on the left side in Fig. 1.

As Fig. 1 illustrates, the differences resulting from comparing modeled results and experimental observations determine the path(s) to model refinements, i.e. by improving the physics models, by collecting and incorporating more data into the existing model, or both. Such iterative comparisons provide continuous feedback into the modeling and UQ process until the differences between the modeled results and experimental observations become sufficiently small.

For complex multi-physics problems like modeling the HSI observables of particulate materials, a hierarchical approach is needed due to limited feasibility of designing and conducting accurate validation and UQ experiments on full-scale systems. To generate comparisons between modeling and experimental results, we apply such a hierarchical approach to designing physical experiments (and/or utilizing available measurement data sets) to compare with the results of predictive computational models. This approach divides a system analysis into several progressively smaller scales— at the system scale (i.e., the full HSI data cube that is acquired by the sensor), at the individual-pixel scale of the data cube, at the micro-scale (i.e. at the level of interaction of electromagnetic radiation with the particulate medium), and also for the intrinsic material properties (i.e., the complex refractive index $n+ik$ of the material, its measurement often requiring the application of models as well) —to identify and quantify measured simulation errors against experimental data and to provide a quantitative assessment of uncertainties. This hierarchy is illustrated in Fig. 2 by the data flow through the different models at different scales. We enable scalability by utilizing both forward and inverse modeling. The left side of Fig. 2 illustrates the forward (up scale) data and model flow from intrinsic optical properties all the way up to the sensor level (data cube). The right hand side of Fig. 2 then starts with the sensor data and propagates the results for materials of interest (MOI) down scale back to the intrinsic properties of the material. This hierarchical approach leverages smaller scale models and data to investigate the accuracy of the various components of the system so that lower-level analysis can inform V/UQ on a larger scale.

The outcome of this V/UQ process will be estimates of input parameter uncertainties for each calibrated model, the confidence range of model output at each scale, and the uncertainty of the overall system response (i.e., sensor data).

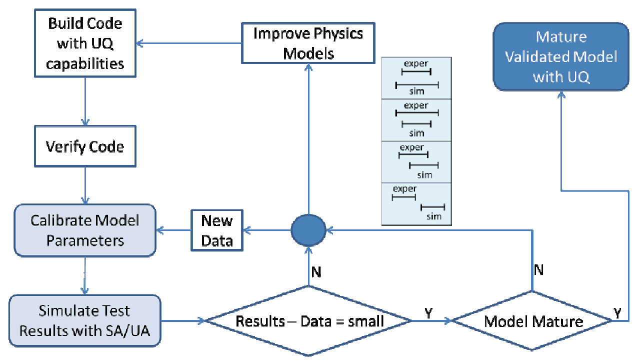

Fig. 1. Model validation process, which includes verification, UQ, and model maturity.

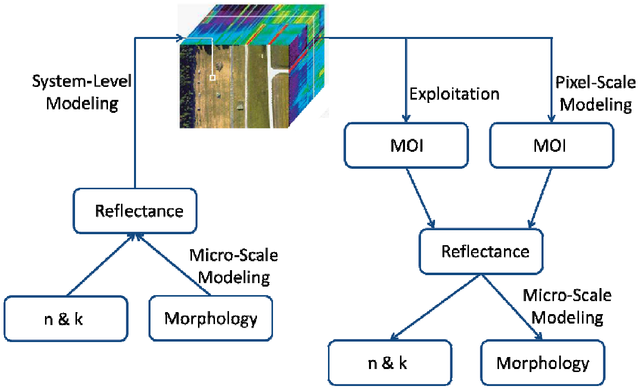

Fig. 2. Data and model flow for the HSI material identification problem.

These estimates will be based on the confidence levels developed in the various decoupled scale problems as well as the upscaling procedure. By considering smaller scale problems that isolate particular aspects of the multi-physics of the full scale system, we should be able to evaluate and isolate the contributions of different aspects of the model to the predictive errors, such as the effects of coupling different physics or the geometric upscaling of the coupled physics. In the following section, we use a micro-scale model to demonstrate the utility of using a lower-level model to inform UQ at a higher level.

MICRO-SCALE MODEL

To illustrate the V/UQ process, we focus the analysis on a single physical scale—the micro-scale. It is well known that the reflectance spectrum of a particulate medium can depend strongly upon the size of the particulates [4], and that the nature of this dependence is a function of the material refractive index. To account for this dependence, we implement a reflectance model developed for an optically thick particulate deposit with corrections for particle packing density and particle shape effects [5]. The model approximates the range of particle size in the deposit with a bimodal volume log-normal [6] particle size distribution (PSD). The analyses performed with the micro-scale model were done using the Dakota software tools [7].

Model Optimization

An optimization analysis was performed on the micro-scale model to estimate the input parameters that best fit laboratory measured fused silica reflectance, with the goal of calibrating model parameters to best approximate material morphology when the material type and the reflectance are known. The micro-scale model utilizes eight input parameters, including:

1) r_g, the characteristic particle radius of the large-particle mode of the PSD
2) $[\ln(\sigma_g)]^2$, the width of the large-particle mode of the PSD
3) r_g, the characteristic particle radius of the small-particle mode of the PSD
4) $[\ln(\sigma_g)]^2$, the width of the small-particle mode of the PSD
5) γ, the population ratio between the two modes
6) particle fill factor to account for the impact of packing density on particle scattering within the medium
7) angle bin # for the angle of incidence, varied to account for surface roughness effects
8) Fresnel-like component resulting from impact of packing density on the first-surface reflection

For an initial assessment of model validity, we focus on the first five parameters associated with the PSD, comparing the PSD calculated from optimized parameters to PSDs measured via laser diffraction. We display one such set of comparisons in Fig. 3. Optimization of the reflectance model to the measurement of a reflectance spectrum of a silica particulate deposit (Fig. 3, left) yields a PSD consistent with independent laser-diffraction measurements of the particle population (Fig. 3, right), demonstrating that the numerically invertible model can extract approximate morphology when material type and reflectance are known.

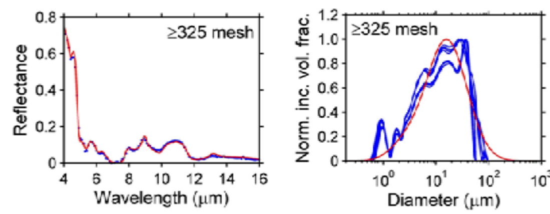

Fig. 3. Results of optimization: left is reflectance and right is particle size distribution.

UNCERTAINTY QUANTIFICATION

The optimization (calibration) exercise discussed above showed that a high level of agreement is obtainable using the micro-scale model results and laboratory data. However, in real world applications, larger uncertainties stemming from multiple sources can be difficult to capture and thus require more complex approaches to modeling uncertainties. Below we describe a stochastic approach to uncertainty modeling.

Bayesian Calibration

To estimate uncertainties with the model input parameters, a Bayesian-like calibration can be used to explicitly deal with (1) treatment of functional output, (2) emulation of the model (functional) output, and (3) calibration parameter screening and selection [8]. In Bayesian calibration, uncertain input parameters are described by a “prior” distribution. The priors are updated with experimental data in a Bayesian framework that involves the experimental data and a likelihood function which describes how well each parameter value is supported by the data. The posterior distribution is the distribution for the input parameters after taking into account the observed data. This posterior distribution can be determined by Bayes' rule [8], as shown in Eq. 1,

$$p(\theta|\, X, \alpha) \propto p(X\,|\theta)\, p(\theta, \alpha) \qquad (1)$$

where the sampling distribution, $p(X|\theta)$, is the distribution of the observed data conditional on its parameters (also called the likelihood function), $p(\theta,\alpha)$ is the prior parameter distributions, and α is a hyper parameter (parameter of the prior distribution). The results of a Bayesian calibration analysis for the same example from the optimization exercise are shown in Fig. 4. The prior distributions are represented by the blue dash lines, the posterior distributions are represented by the histograms, with a beta distribution being fit to each histogram (red curves).

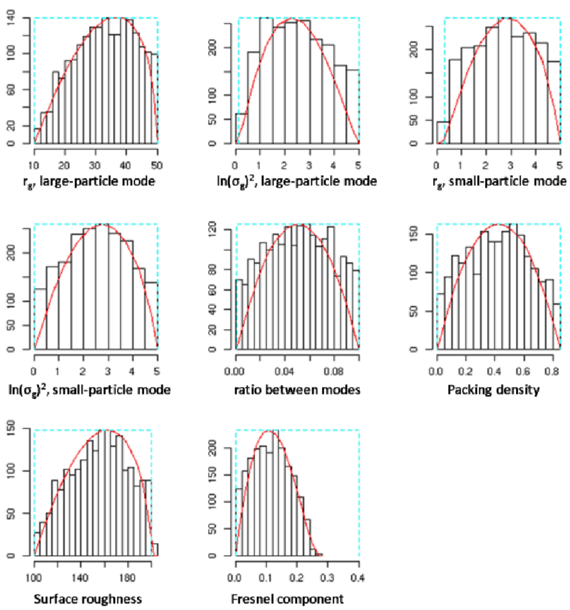

Fig. 4. **C**alibration results: blue dash lines are prior distributions, histograms are posterior distributions and red curves are beta distributions fit to the histograms..

For this analysis, 150 functional evaluations were performed using the prior distributions shown in Fig. 4 and a Latin Hypercube sampling design [9]. A Gaussian Process (GP) model was then fit to the functional evaluations to be used as a surrogate model (emulator). A Markov Chain Monte Carlo analysis with 5000 iterations was then performed using the GP model to best fit the measured data [10].

Sensitivity Analysis

After calibration, a sensitivity analysis (SA) was performed to further understand the model, i.e., to ascertain which model parameters contribute the most to the uncertainty in the output, and to ensure that the model behaves as expected when model parameters vary [11]. A simple SA was performed using the posterior distributions from the calibration and the Morris design [12]. In this design, only one parameter value is changed and the model is run. A compilation of this analysis is shown in Fig. 5.

The SA utilized a very simple designed, nonetheless revealed added insights. For instance, changing values for parameters 3-5 had very little effect on reflectance, indicating that the primary impact of particle size is associated with the large particle mode of the PSD. While changes in parameters 1, 2, 6, and 7 had noticeable effects on the change in reflectance, the change in parameter 8 had a much larger effect. This is consistent with the reported strong impact of particle packing density on changes in the reflectance due to the Fresnel-like component [13]. The analysis also pointed to anomalous model results when the packing density (parameter 6) was large for wavelengths between 5-6 µm (green curve), likely associated with a limited range of numerical applicability in the computation used to account for the impact of packing density on particle scattering within the medium.

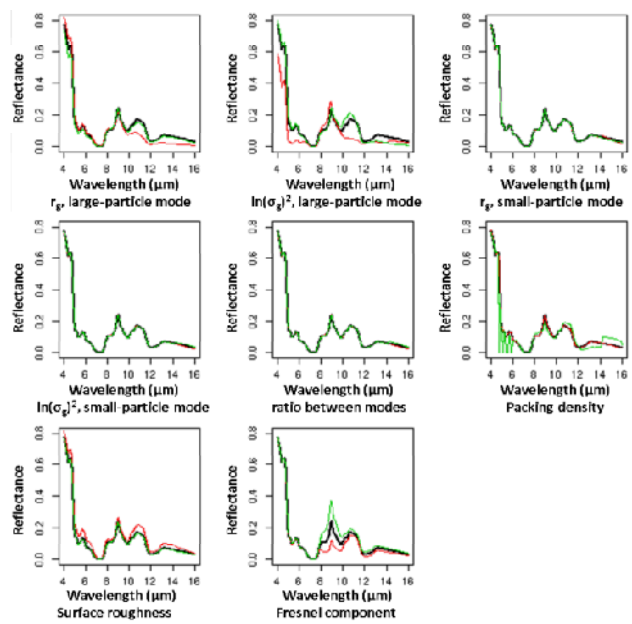

Fig. 5. Sensitivity analysis utilizing the Morris design for global sensitivity.

Uncertainty Analysis

Uncertainty analysis (UA) refers to the process of propagating the uncertainty in the model parameters through to the outputs of interest to obtain a distribution of model output. Utilizing the posterior parameter distributions extracted from the calibration exercise, a Monte Carlo simulation was performed to estimate the output uncertainties. The results of the UA are shown in Fig. 6. Importantly, these uncertainties assume both the PSD and the Fresnel-like component are unknown, so the results emphasize the impact of these parameters on the HSI observable. These results could then be used to propagate up the modeling hierarchy as illustrated in Fig. 6 to

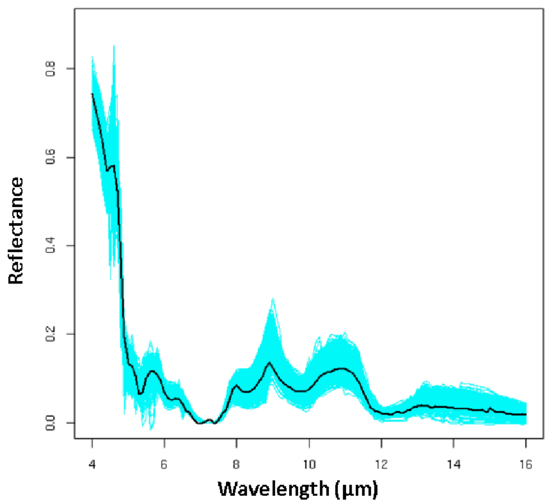

Fig. 6. Uncertainty analysis based on the calibration posterior parameter distributions assuming no known parameters.

investigate how uncertainties at the micro-scale could affect modeling results at the system (i.e. sensor data) level.

CONCLUSION

In this paper, we introduce a hierarchical approach to validating a multi-scale model for predicting HSI observables from solid particulate materials, and illustrate techniques for quantifying uncertainties in the complex modeling process. We describe an iterative process of using comparative differences between experimental observations and model results to evaluate model validity. Using a single-scale model as a proof-of-concept example, we demonstrate the feasibility of the Bayesian approach to modeling uncertainty at the micro scale and briefly discuss using the results for estimating its impact on model uncertainty at higher scales. We also show that sensitivity and uncertainty analysis, as part of our approach, generated added insight into anomalies in the modeling, which can provide valuable feedback to model developers and experimentalists. Our work helps address UQ within the HSI model application domain and, with continuing efforts, will help researchers and stakeholders gain greater confidence in the utility and defensibility of multi-scale physical models and model outputs.

ACKNOWLEDGEMENT

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